STIC Search Report
Biotech-Chem Library

STIC Database Tracking Number: 155417

TO: Tamthom Troung **Location: REM/5C18** **Art Unit: 1624** June 23, 2005 **Case Serial Number: 10/725657**	**From: P. Sheppard** **Location: Remsen Building** **Phone: (571) 272-2529** **sheppard@uspto.gov**

Search Notes

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FILE 'HCAPLUS' ENTERED AT 12:53:36 ON 23 JUN 2005
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FILE COVERS 1907 - 23 Jun 2005  VOL 142 ISS 26
FILE LAST UPDATED: 22 Jun 2005  (20050622/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

 This file contains CAS Registry Numbers for easy and accurate
 substance identification.

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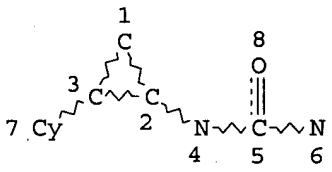


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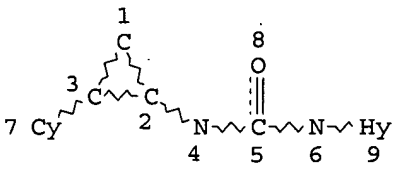


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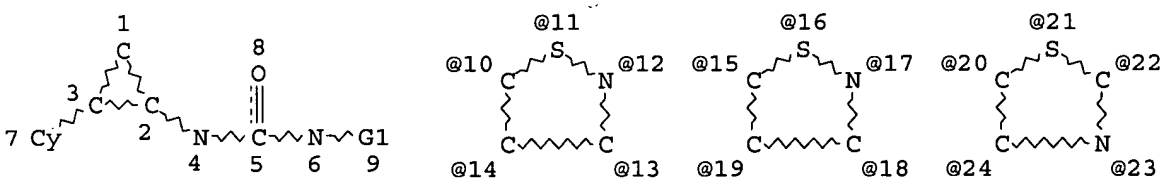

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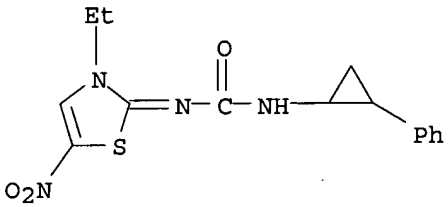
L14 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1972:547456 HCAPLUS
DOCUMENT NUMBER: 77:147456
TITLE: 1-Alkyl-3-(3-alkyl-5-nitro-4-thiazolin-2-ylidene)ureas and related compounds as schistosomicides
AUTHOR(S): Werbel, Leslie M.; Degnan, Margaret B.; Harger, Gail F.; Capps, David B.; Islip, Peter J.; Closier, Michael D.
CORPORATE SOURCE: Res. Dev. Div., Parke, Davis and Co., Ann Arbor, MI, USA
SOURCE: Journal of Medicinal Chemistry (1972), 15(9), 955-63
CODEN: JMCMAR; ISSN: 0022-2623
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Many 1-alkyl-3-[3-(alkyl or aralkyl)-5-nitro-4-thiazolin-2-ylidene]ureas (analogs of niridazole) were curative against Schistosoma mansoni in mice, and several were curative in rhesus monkeys but not tolerated by dogs. Among the most active compds. tested was 1-ethyl-3-(3-benzyl-5-nitro-4-thiazoline-2-ylidene)urea (I) [26231-01-6], which was curative at 100 mg/kg/day for 5 days by gavage in mice and at a similar dosage in monkeys. Structure-activity relations were discussed. To synthesize I,

2-amino-5-nitrothiazole was reacted with EtNCO to form 1-ethyl-3-(5-nitro-2-thiazolyl)urea, which was then reacted with BzI in the presence of NaH.

IT **38908-70-2**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(schistosomicidal activity of)

RN 38908-70-2 HCAPLUS

CN Urea, (3-ethyl-5-nitro-2(3H)-thiazolylidene)(2-phenylcyclopropyl)- (9CI) (CA INDEX NAME)



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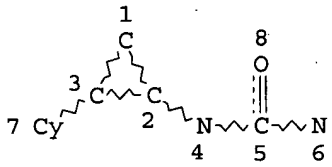

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DEFAULT ECLEVEL IS LIMITED

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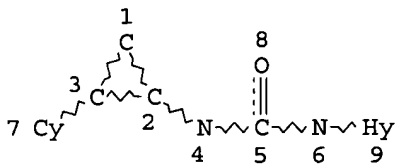

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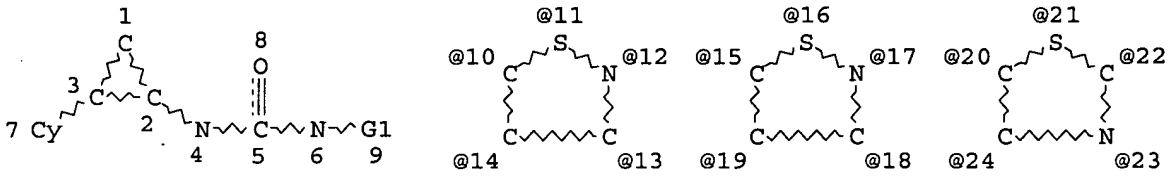

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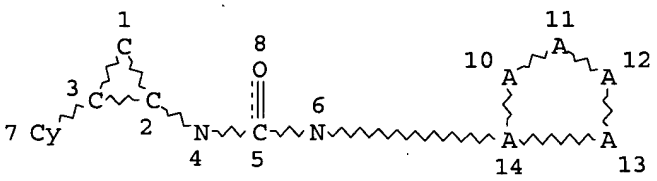

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STEREO ATTRIBUTES: NONE
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L17 ANSWER 1 OF 5 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2004:902086 HCAPLUS
DOCUMENT NUMBER: 141:388753
TITLE: Heterocyclic compound modulators of Tie-2 and other kinases, and therapeutic use
INVENTOR(S): Chen, Jeff; Dalrymple, Lisa; Epshteyn, Sergery;

Forsyth, Timothy; Huynh, Tai; Leahy, James; Mann, Grace; Mann, Larry W.; Ridgway, Brian; Sangalang, Joan C.; Takeuchi, Craig
PATENT ASSIGNEE(S): Exelixis, Inc., USA
SOURCE: PCT Int. Appl., 126 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004091480	A2	20041028	WO 2004-US10626	20040408

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

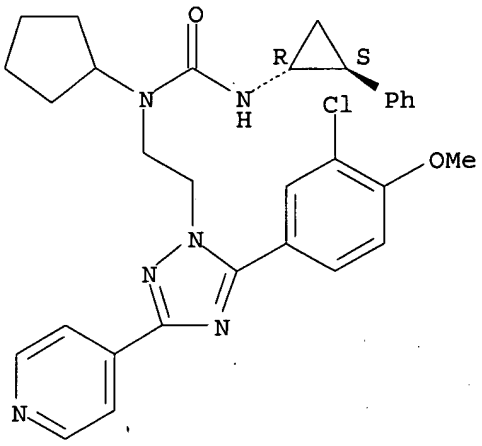
PRIORITY APPLN. INFO.: US 2003-461471P P 20030409
OTHER SOURCE(S): MARPAT 141:388753
AB The invention provides heterocyclic compds. for modulating protein kinase enzymic activity for modulating cellular activities such as proliferation, differentiation, programmed cell death, migration and chemoinvasion. Compds. of the invention inhibit, regulate and/or modulate kinases, particularly Tie-2. Methods of using the compds. and pharmaceutical compns. thereof to treat kinase-dependent diseases and conditions are also an aspect of the invention. Preparation of triazolyl compds. of the invention is included.

IT **783327-32-2**
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(heterocyclic compound modulators of Tie-2 and other kinases, and therapeutic use)

RN 783327-32-2 HCAPLUS

CN Urea, N-[2-[5-(3-chloro-4-methoxyphenyl)-3-(4-pyridinyl)-1H-1,2,4-triazol-1-yl]ethyl]-N-cyclopentyl-N'-[(1R,2S)-2-phenylcyclopropyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L17 ANSWER 2 OF 5 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2004:780696 HCAPLUS
DOCUMENT NUMBER: 141:295849
TITLE: Preparation of carboxamidopyrrolidines as melanin-concentrating hormone receptor antagonists and compositions and methods related thereto
INVENTOR(S): Goodfellow, Val; Rowbottom, Martin; Dyck, Brian P.; Tamiya, Junko; Zhang, Mingzhu; Grey, Jonathan; Vickers, Troy D.
PATENT ASSIGNEE(S): Neurocrine Biosciences, Inc., USA
SOURCE: PCT Int. Appl., 180 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004081005	A1	20040923	WO 2004-US7259	20040308

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: US 2003-452776P P 20030307
US 2003-518265P P 20031107
OTHER SOURCE(S): MARPAT 141:295849
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

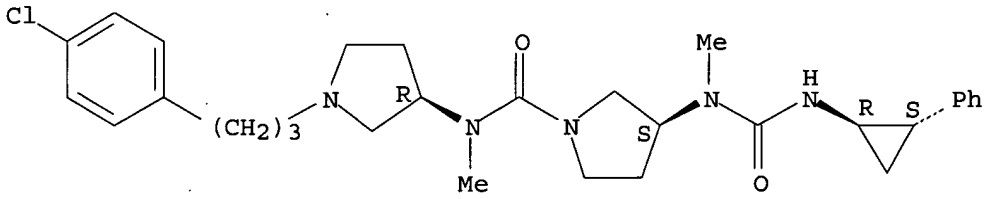
AB Title compds. I [m = 0 or 1; n = 1 or 2; X = -CH2-, or -N(R6)-; R1 = H, (un)substituted-alkyl, -aryl, -arylalkyl, etc.; R2 and R5 independently = H, (un)substituted alkyl; R3 = H, (un)substituted-alkyl, -arylalkyl, -heteroarylalkyl; R4 = (un)substituted-alkyl, -aryl, -heterocycle; R6 = H or (un)substituted alkyl] and their pharmaceutically acceptable salt, are disclosed as melanin-concentrating hormone (MCH) receptor antagonists having utility for the treatment of MCH receptor-based disorders such as obesity. Thus, e.g., II was prepared via amidation of of III (preparation given) with benzoyl chloride. Methods for evaluation of compds. are described (no data). Also disclosed are compns. containing a compound of this invention, as well as methods relating to the use thereof.

IT **762278-96-6P 762279-03-8P 762279-04-9P**
762279-05-0P 762279-06-1P 762284-01-5P
762284-02-6P 762284-03-7P 763130-70-7P
763131-31-3P 763131-32-4P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate; preparation of carboxamidopyrrolidine derivs. as melanin-concentrating hormone receptor antagonists)

RN 762278-96-6 HCAPLUS

CN 1-Pyrrolidinecarboxamide, N-[(3R)-1-[3-(4-chlorophenyl)propyl]-3-pyrrolidinyl]-N-methyl-3-[methyl[[[(1R,2S)-2-phenylcyclopropyl]amino]carbonyl]amino]-, (3S)- (9CI) (CA INDEX NAME)

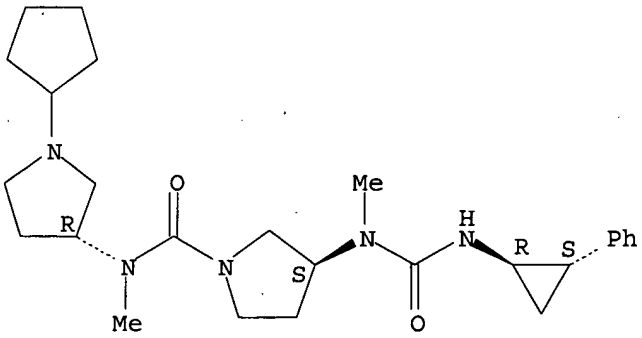
Absolute stereochemistry.



RN 762279-03-8 HCAPLUS

CN 1-Pyrrolidinecarboxamide, N-[(3R)-1-cyclopentyl-3-pyrrolidinyl]-N-methyl-3-[methyl[[[(1R,2S)-2-phenylcyclopropyl]amino]carbonyl]amino]-, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

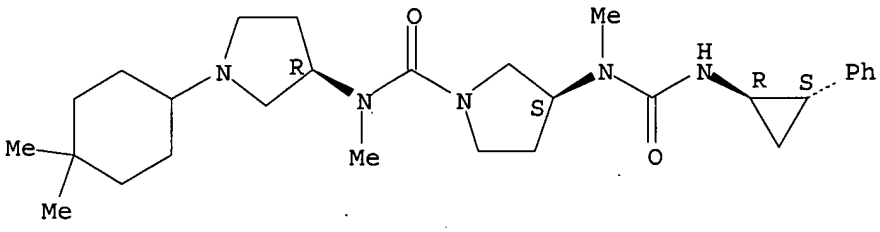


RN 762279-04-9 HCAPLUS

CN 1-Pyrrolidinecarboxamide, N-[(3R)-1-(4,4-dimethylcyclohexyl)-3-

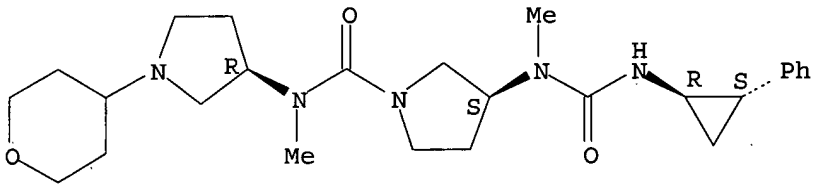
pyrrolidinyl]-N-methyl-3-[methyl[[[(1R,2S)-2-phenylcyclopropyl]amino]carbonyl]amino]-, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



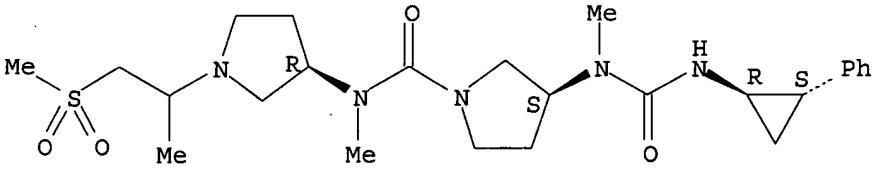
RN 762279-05-0 HCAPLUS
CN 1-Pyrrolidinecarboxamide, N-methyl-3-[methyl[[[(1R,2S)-2-phenylcyclopropyl]amino]carbonyl]amino]-N-[(3R)-1-(tetrahydro-2H-pyran-4-yl)-3-pyrrolidinyl]-, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 762279-06-1 HCAPLUS
CN 1-Pyrrolidinecarboxamide, N-methyl-N-[(3R)-1-[1-methyl-2-(methylsulfonyl)ethyl]-3-pyrrolidinyl]-3-[methyl[[[(1R,2S)-2-phenylcyclopropyl]amino]carbonyl]amino]-, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 762284-01-5 HCAPLUS
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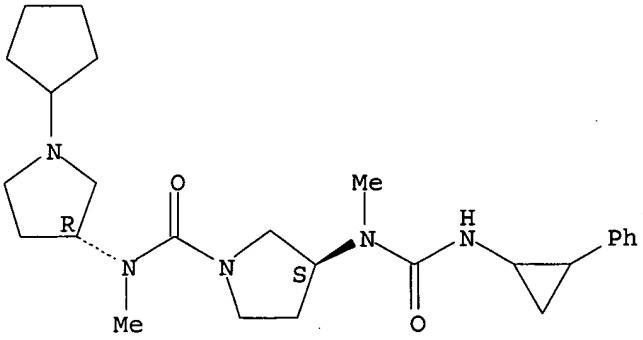
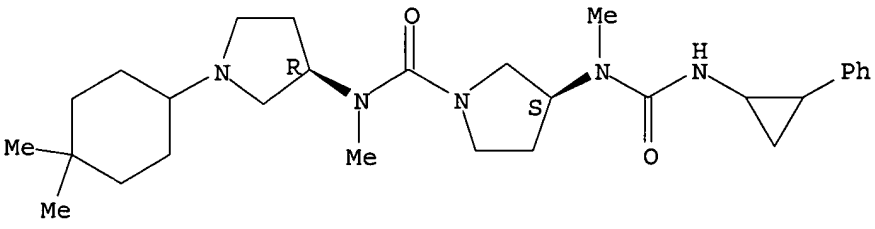
Absolute stereochemistry.



RN 762284-02-6 HCAPLUS
CN 1-Pyrrolidinecarboxamide, N-[(3R)-1-(4,4-dimethylcyclohexyl)-3-pyrrolidinyl]-N-methyl-3-[methyl[[(2-phenylcyclopropyl)amino]carbonyl]amino]-, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



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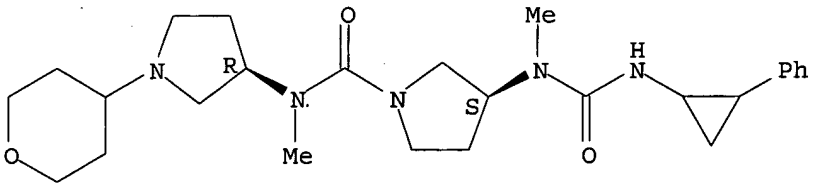
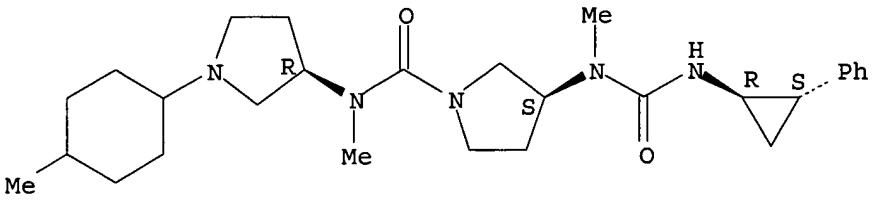
Absolute stereochemistry.



RN 763130-70-7 HCAPLUS
CN 1-Pyrrolidinecarboxamide, N-methyl-N-[(3R)-1-(4-methylcyclohexyl)-3-pyrrolidinyl]-3-[methyl[[[(1R,2S)-2-phenylcyclopropyl]amino]carbonyl]amino]-, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 763131-31-3 HCAPLUS
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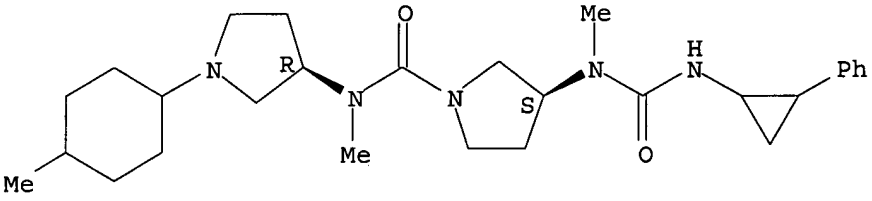
CRN 763131-30-2
CMF C28 H43 N5 O2

Absolute stereochemistry.



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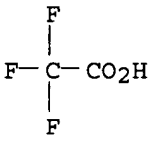
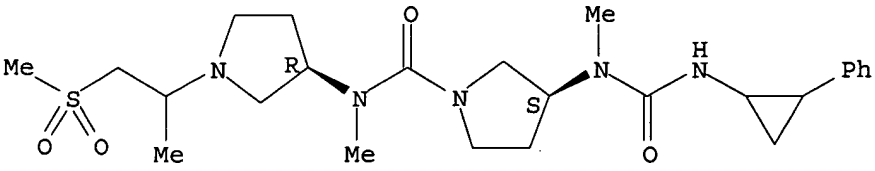


RN 763131-32-4 HCAPLUS
CN 1-Pyrrolidinecarboxamide, N-methyl-N-[(3R)-1-[1-methyl-2-(methylsulfonyl)ethyl]-3-pyrrolidinyl]-3-[methyl[[(2-phenylcyclopropyl)amino]carbonyl]amino]-, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



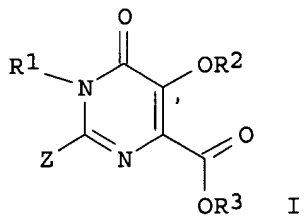
REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 3 OF 5 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2003:591157 HCAPLUS
DOCUMENT NUMBER: 139:149641
TITLE: Preparation of pyrimidinones as viral polymerase inhibitors
INVENTOR(S): Avolio, Salvatore; Colarusso, Stefania; Conte, Immacolata; Harper, Steven; Koch, Uwe; Malancona, Savina; Matassa, Victor Giulio; Narjes, Frank; Petrocchi, Alessia; Summa, Vincenzo
PATENT ASSIGNEE(S): Istituto Di Ricerche Di Biologia Molecolare P. Angeletti Spa, Italy
SOURCE: PCT Int. Appl., 82 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

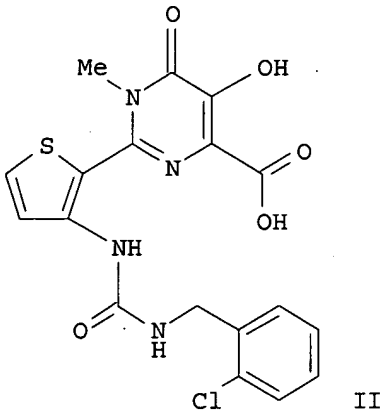
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003062211	A1	20030731	WO 2003-GB124	20030115
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2473508	AA	20030731	CA 2003-2473508	20030115
EP 1470113	A1	20041027	EP 2003-700366	20030115
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
US 2005130997	A1	20050616	US 2003-500971	20030115

PRIORITY APPLN. INFO.: GB 2002-1179 A 20020118
WO 2003-GB124 W 20030115

OTHER SOURCE(S): MARPAT 139:149641
GI



I



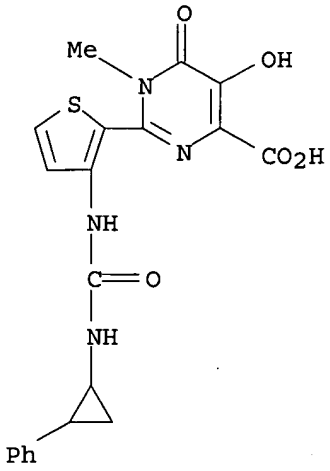
II

AB Title compds. I [wherein Z = (un)substituted alkynyl, aryl, or heteroaryl; R1 = (un)substituted alkyl or (aryl)alkyl; R2 = H, (un)substituted alkyl, alkylcarbonyl, aryl, arylcarbonyl, heteroaryl, (aryl)alkyl, (heteroaryl)alkyl; R3 = H, alkyl, (heterocycloalkyl)alkyl, dialkylaminoalkyl, (alkylcarbonyloxy)alkyl, (cycloalkoxycarbonyloxy)alkyl; and their pharmaceutically acceptable salts] were prepared as inhibitors of viral polymerases, especially the hepatitis C virus (HCV) polymerase enzyme. For example, II was prepared from 3-nitrothiophene-2-carbonitrile (preparation given) by base-catalyzed nucleophilic addition of hydroxylamine, reaction with di-Me acetylenedicarboxylate in CH2Cl2, intramol. cyclocondensation in xylene, room temperature O-acylation with pivaloyl chloride in the presence of 4-DMAP, base-catalyzed N-methylation with di-Me sulfate for 1 h, hydrogenation over Pd/C, and reaction with ortho-chlorobenzyl isocyanate in dichloromethane. I exhibited an IC50 value of 100 μM or less for inhibition of HCV polymerase. Thus, I and their pharmaceutical compns. are useful for treating or preventing an illness due to HCV (no data).

IT **572917-01-2P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(viral polymerase inhibitor; preparation of pyrimidinones as viral polymerase inhibitors)

RN 572917-01-2 HCAPLUS

CN 4-Pyrimidinecarboxylic acid, 1,6-dihydro-5-hydroxy-1-methyl-6-oxo-2-[3-[[[(2-phenylcyclopropyl)amino]carbonyl]amino]-2-thienyl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 4 OF 5 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2002:465982 HCAPLUS
DOCUMENT NUMBER: 137:47213
TITLE: Preparation of fused pyrimidinones and benzodioxaborolidinylpropylaminopyrrolo[1,2-a]pyrimidines as inhibitors of hepatitis C ns3 protease for the treatment of hepatitis C and other viral diseases
INVENTOR(S): Glunz, Peter W.; Douty, Brent D.; Han, Wei
PATENT ASSIGNEE(S): Bristol-Myers Squibb Pharma Company, USA
SOURCE: PCT Int. Appl., 270 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002048116	A2	20020620	WO 2001-US47911	20011212
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2002030763	A5	20020624	AU 2002-30763	20011212
US 2003064962	A1	20030403	US 2001-15304	20011212
US 6653295	B2	20031125		

PRIORITY APPLN. INFO.: US 2000-255290P P 20001213
WO 2001-US47911 W 20011212

OTHER SOURCE(S): MARPAT 137:47213
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

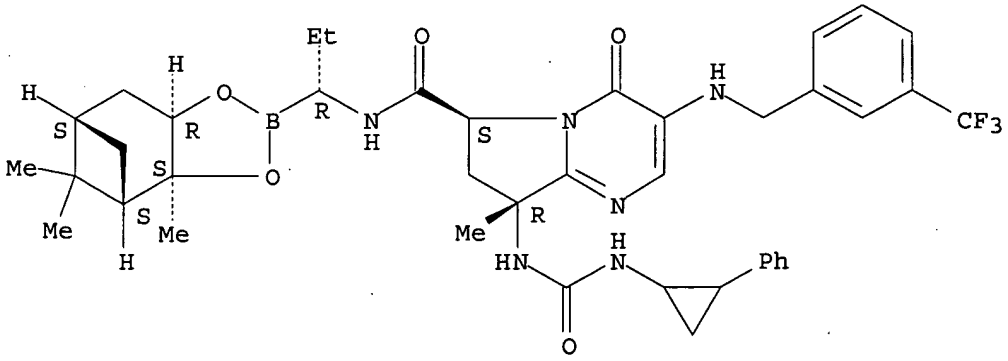
AB Fused pyrimidinones I [A1 = (un)substituted CH2, CH2CH2, CH2CH2CH2, A2CH2, A2CH2CH2, CH2A2CH2; A2 = O, S, (un)substituted imino; A3 = H, R9CO, R9O, R9S, R9CONH, R9NHCO, etc.; W = (un)substituted boronic acid ester, QCOCO, QNHCOCO, QOCOCO, QNHCOCF2CO, COQ3, F3CCO, F3CCF2CO, OHC, amino acid residue; Q3 = (un)substituted aryl, heterocyclyl; R1 = H, F, (un)substituted alkyl, alkenyl, alkynyl, cycloalkyl; R2 = H, alkyl; Q, R3, R9 = (un)substituted alkyl, alkenyl, alkynyl, cycloalkyl, aryl, heterocyclyl; R6, R13 = H, (un)substituted alkyl, alkenyl, alkynyl, cycloalkyl, aryl, aralkyl, cycloalkylalkyl; R3R13 = (un)substituted carbocyclic ring, alkylidene] and particularly dioxaborolylpropylamino pyrrolopyriminecarboxamides such as II are prepared as inhibitors of hepatitis C viral protein ns3 protease for the treatment of hepatitis C and other viral diseases. E.g., esterification of L-pyroglutamic acid with AcOCMe3 and HClO4, thionation with Lawesson's reagent, S-methylation with MeI, and amidation with NH4Cl gives nonracemic aminopyrrolinecarboxylate III. Treatment of III with di-Me 2-(methoxymethylene)malonate, hydrolysis of the Me ester moiety with LiOH, preparation of the acyl azide with diphenylphosphoryl azide and Curtius rearrangement in the presence of PhCH2OH, and hydrolysis of the tert-Bu ester with CF3CO2H gives pyrrolo[1,2-a]pyrimidine IV. Coupling of IV with an α-allyl aminomethylboronate pinanediol ester gives II. I inhibit hepatitis C ns3 protease with IC50 values of <100 μM. Pharmaceutical compns. containing I are given.

IT **437758-67-3P 437758-68-4P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(invention compd; preparation of fused pyrimidinones and benzodioxaborolidinylpropylaminopyrrolo[1,2-a]pyrimidines as inhibitors of hepatitis C ns3 protease for the treatment of hepatitis C and other viral diseases)

RN 437758-67-3 HCAPLUS

CN Pyrrolo[1,2-a]pyrimidine-6-carboxamide, N-[(1R)-1-[(3aS,4S,6S,7aR)-hexahydro-3a,5,5-trimethyl-4,6-methano-1,3,2-benzodioxaborol-2-yl]propyl]-4,6,7,8-tetrahydro-8-methyl-4-oxo-8-[[[(2-phenylcyclopropyl)amino]carbonyl]amino]-3-[[[3-(trifluoromethyl)phenyl]methyl]amino]-, (6S,8R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

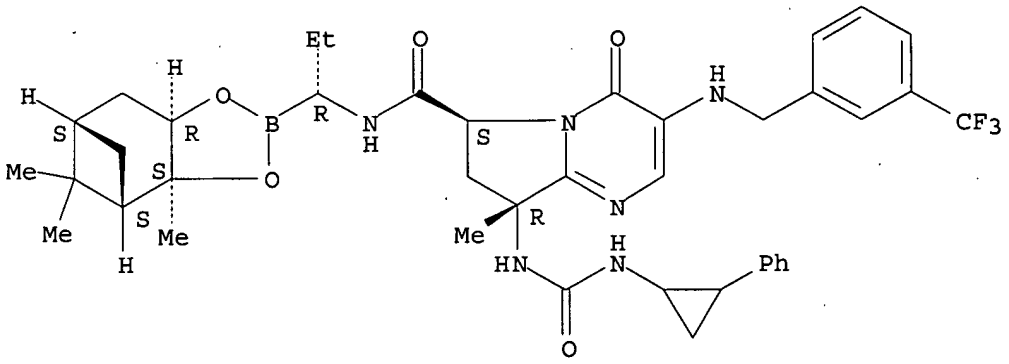


RN 437758-68-4 HCAPLUS
CN Pyrrolo[1,2-a]pyrimidine-6-carboxamide, N-[(1R)-1-[(3aS,4S,6S,7aR)-hexahydro-3a,5,5-trimethyl-4,6-methano-1,3,2-benzodioxaborol-2-yl]propyl]-4,6,7,8-tetrahydro-8-methyl-4-oxo-8-[[[(2-phenylcyclopropyl)amino]carbonyl]amino]-3-[[[3-(trifluoromethyl)phenyl]methyl]amino]-, (6S,8R)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

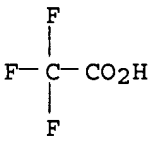
CRN 437758-67-3
CMF C40 H48 B F3 N6 O5

Absolute stereochemistry.



CM 2

CRN 76-05-1
CMF C2 H F3 O2



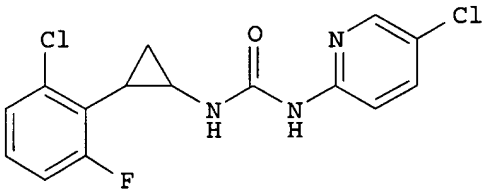
L17 ANSWER 5 OF 5 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1995:789162 HCAPLUS
DOCUMENT NUMBER: 123:198634
TITLE: Preparation of N-[aryl(cyclo)alkyl)-N'-pyridylureas and analogs as HIV reverse transcriptase inhibitors
INVENTOR(S): Lind, Peter Thomas; Noreen, Rolf; Morin, John Michael; Ternansky, Robert John
PATENT ASSIGNEE(S): Medivir AB, Swed.
SOURCE: PCT Int. Appl., 104 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE

WO 9506034	A1	19950302	WO 1994-US9406	19940824
W: AT, AU, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, ES, FI, GB, HU, JP, KP, KR, KZ, LK, LU, LV, MG, MN, MW, NL, NO, NZ, PL, PT, RO, RU, SD, SE, SK, UA, US, UZ, VN				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
CA 2168447	AA	19950302	CA 1994-2168447	19940824
AU 9477153	A1	19950321	AU 1994-77153	19940824
AU 687440	B2	19980226		
EP 706514	A1	19960417	EP 1994-927932	19940824
EP 706514	B1	19981118		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE				
JP 09502702	T2	19970318	JP 1994-507689	19940824
AT 173466	E	19981215	AT 1994-927932	19940824
ES 2123156	T3	19990101	ES 1994-927932	19940824
NZ 273741	A	20000623	NZ 1994-273741	19940824
US 5849769	A	19981215	US 1996-601030	19960503
US 6376492	B1	20020423	US 2000-567857	20000509
US 2002132794	A1	20020919	US 2002-76163	20020213
US 2004116418	A1	20040617	US 2003-725657	20031201
PRIORITY APPLN. INFO.:			US 1993-110956 A	19930824
			WO 1994-US9406 W	19940824
			US 1996-601030 A3	19960503
			US 1998-114935 B1	19980714
			US 2000-567857 A3	20000509
			US 2002-76163 A3	20020213

OTHER SOURCE(S): MARPAT 123:198634

GI



I

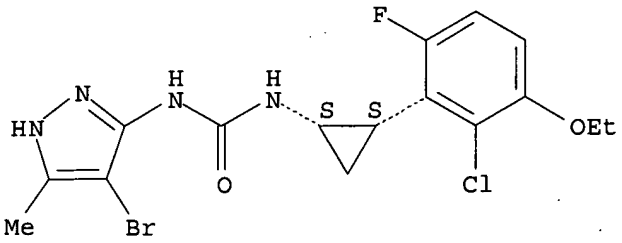
AB R2R4NZNR1R3 [R1 = (heterocyclic) organic ring residue; R2 = CR7R9CR5R6R8; R3,R4 = H, OH, alk(en)yl, CONH2, etc.; R5 = groups cited for R1, NH2, OH, alkoxy, etc.; R6-R9 = H, (cyclo)alkyl, halo, NH2, CO2H, etc.; Z = CO, C(:NH), C(:CH2), SO2, etc.] were prepared Thus, cis-2-(2-chloro-6-fluorophenyl)cyclopropylisocyanate (preparation from 2-chloro-6-fluorobenzaldehyde given) was condensed with 2-amino-5-chloropyridine to give title compound cis-I which had IC50 of 0.0004μg/mL against HIV reverse transcriptase in vitro.

IT **167683-23-0P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of N-[aryl(cyclo)alkyl)-N'-pyridylureas and analogs as HIV reverse transcriptase inhibitors)

RN 167683-23-0 HCAPLUS

CN Urea, N-(4-bromo-5-methyl-1H-pyrazol-3-yl)-N'-[2-(2-chloro-3-ethoxy-6-fluorophenyl)cyclopropyl]-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



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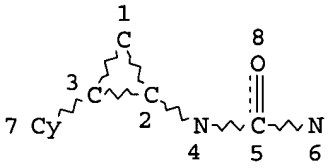
L1 STR



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DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 8

STEREO ATTRIBUTES: NONE
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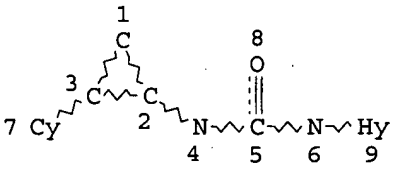
L4 STR



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DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
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NUMBER OF NODES IS 9

STEREO ATTRIBUTES: NONE
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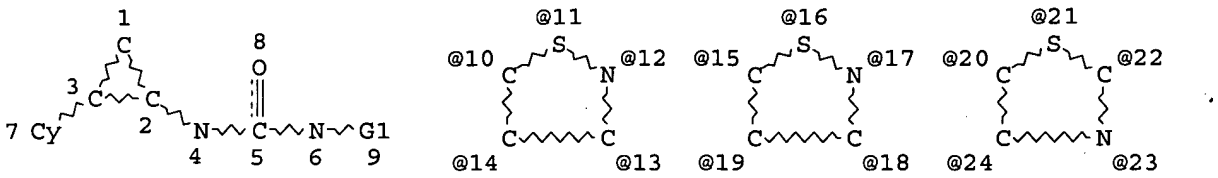
L10 STR



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DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 24

STEREO ATTRIBUTES: NONE
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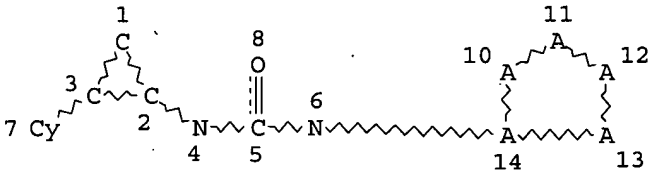
L12 STR



NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
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NUMBER OF NODES IS 13

STEREO ATTRIBUTES: NONE
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L14 1 SEA FILE=HCAPLUS ABB=ON PLU=ON L11
L15 17 SEA FILE=REGISTRY ABB=ON PLU=ON L13 NOT L11
L16 5 SEA FILE=HCAPLUS ABB=ON PLU=ON L15
L17 5 SEA FILE=HCAPLUS ABB=ON PLU=ON L16 NOT L14
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L20 30 SEA FILE=HCAPLUS ABB=ON PLU=ON L19 NOT (L14 OR L17)
L21 2 SEA FILE=HCAPLUS ABB=ON PLU=ON L20 AND PD=<AUGUST 24, 1994

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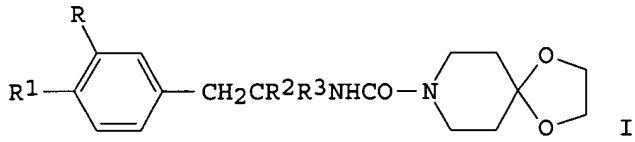
L21 ANSWER 1 OF 2 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1978:74324 HCAPLUS
DOCUMENT NUMBER: 88:74324
TITLE: Psychoactive agents. IV. Synthesis and CNS depressant activity of some β-arylethyl- and β-styrylureas

AUTHOR(S): Arya, V. P.; David, J.; Grewal, R. S.
CORPORATE SOURCE: Ciba-Geigy Res. Cent., Bombay, India
SOURCE: Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry (1977), 15B(7), 635-40
CODEN: IJSBDB; ISSN: 0376-4699
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 88:74324

GI



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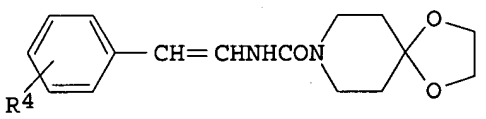
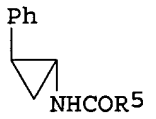


II



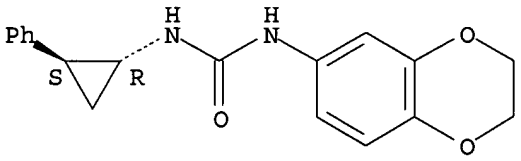
III

AB Treatment of 3,4-RR1C6H3CH2CR2R3NH2 (R = H, MeO; R1 = H, MeO, Cl, F; R2, R3 = H, Me) with COCl2 gave 3,4-RR1C6H3CH2CR2R3NCO, which reacted with 8-aza-1,4-dioxaspiro[4.5]decane to give the ureas I. Styrylureas II (R4 = H, Cl, F) and (phenylcyclopropyl)ureas III [R5 = Q-Q3, 4-hydroxy-4-(4-fluorophenyl)piperidino, (hexahydroazepin-1-yl)amino, ClCH2CH2CH2NH] were prepared similarly. (Arylethyl)ureas were prepared from 9-aza-3,3-dimethyl-1,5-dioxaspiro[5.5]undecane, 9-aza-1,4-dioxaspiro[4.5]decane, 1-azaspiro[4.5]decane and 3-azaspiro[5.5]undecane. The central nervous system (CNS) depressant and anticonvulsant activity of these compds. were reported.

IT **65535-80-0P 65535-81-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

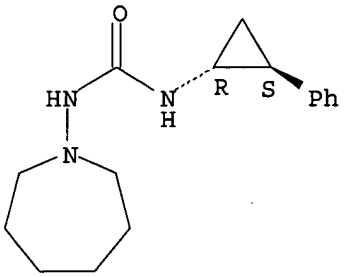
RN 65535-80-0 HCAPLUS
CN Urea, N-(2,3-dihydro-1,4-benzodioxin-6-yl)-N'-(2-phenylcyclopropyl)-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 65535-81-1 HCAPLUS
CN Urea, N-(hexahydro-1H-azepin-1-yl)-N'-(2-phenylcyclopropyl)-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L21 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1966:468519 HCAPLUS
DOCUMENT NUMBER: 65:68519
ORIGINAL REFERENCE NO.: 65:12792c-e
TITLE: Cytokinin activity of some substituted ureas and thioureas
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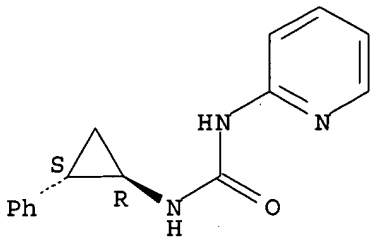
CORPORATE SOURCE: Div. Plant Ind., C.S.I.R.O., Canberra, Australia
SOURCE: Proc. Roy. Soc. (London), Ser. B. (**1966**), 165(999), 245-65
DOCUMENT TYPE: Journal
LANGUAGE: English

AB N,N'-Diphenylurea had reproducible cytokinin activity. N-Monosubstituted and N,N'-disubstituted ureas (500) were examined, and .apprx.250 were active. The following generalizations were made with regard to the correlation of chemical structure with biol. activity: (1) phenylurea was the simplest active compound; (2) an HNCONH bridge conferred higher activity than an HNCSNH bridge; (3) compds. in which both amino H atoms on 1 or both sides of the bridge were substituted were of low activity or were inactive; (4) ring substitution on the bridge (RNHCONH2, R = substituted phenyl ring) increased the activity, and meta substitutions gave highest activity, while ortho substitutions gave lowest activity; (5) compds. with electron-attracting substituents were more active than those with electron-donating substituents; (6) pyridyl compds. were active, but compds. with non-planar rings were inactive; and (7) in compds. of the type RNHCONHR', where R and R' were phenyl or substituted phenyl groups, compds. having 1 unsubstituted phenyl ring had higher activities than those having 2 substituted phenyl groups. Some ureas showed detectable activity at 0.1 ppm., which was .apprx.4-fold less active than kinetin in the tobacco pith assay.

IT **13257-07-3**, Urea, 1-(2-phenylcyclopropyl)-3-(2-pyridyl)-, trans- (plant regulator activity of)
RN 13257-07-3 HCAPLUS
CN Urea, 1-(2-phenylcyclopropyl)-3-(2-pyridyl)-, trans- (8CI) (CA INDEX NAME)

Relative stereochemistry.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